Green's Function Monte Carlo Calculations of Light Nuclei with Two- and Three-Nucleon Interactions from Chiral Effective Field Theory

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with
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International Collaborations in Nuclear Theory: Theory for open-shell nuclei near the limits of stability

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   - *Ab-Initio* Calculations of Nuclei - GFMC
   - Nuclear Interactions
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3. NNN Interaction and Fits
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   - Future Work
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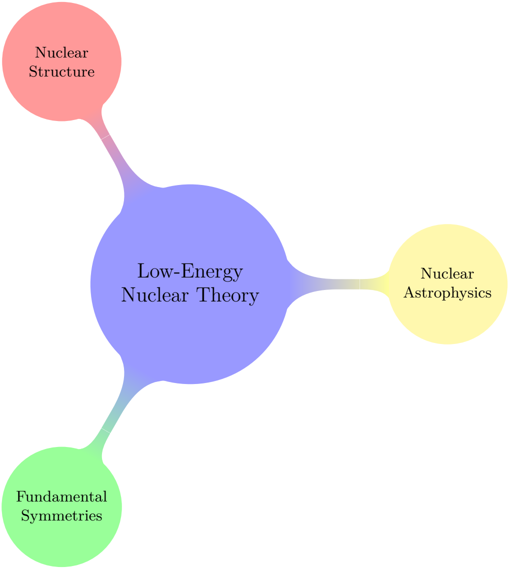
Motivation

Big Questions

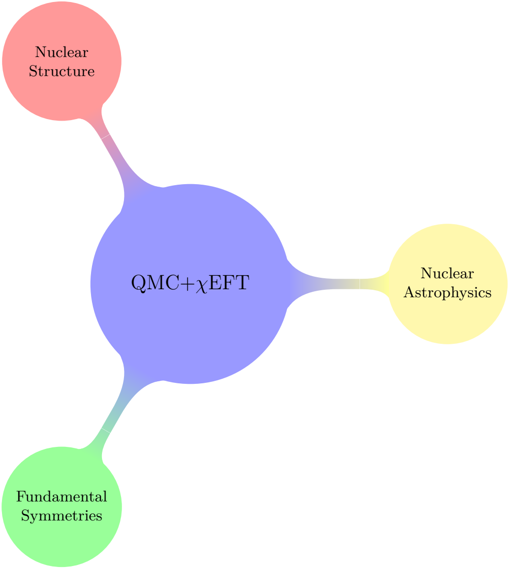
Low-energy nuclear theory connects several research areas in physics.



Motivation

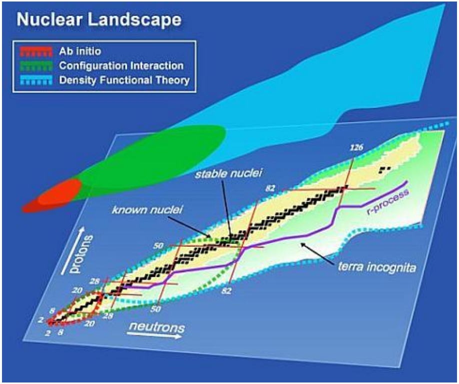
Big Questions

Low-energy nuclear theory connects several research areas in physics. QMC+χEFT is a compelling piece of the puzzle.



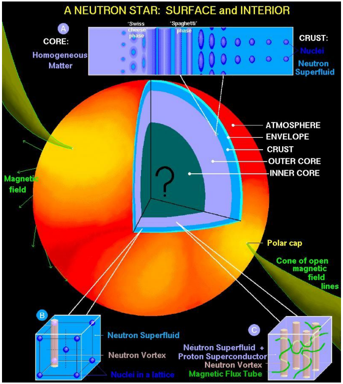
Nuclear Structure

- What are the limits of nuclear existence?
- How far can we push *ab initio* calculations?
- How can we build a coherent framework for describing nuclei, nuclear matter, and nuclear reactions?
  This talk: GFMC+χEFT



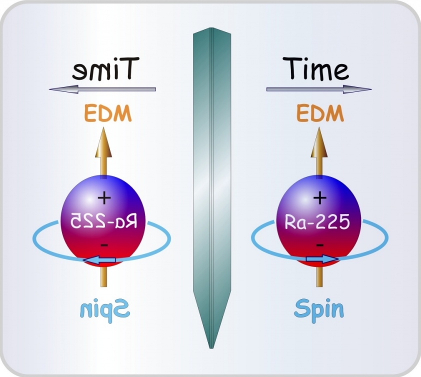
Nuclear Astrophysics

- How did the elements come into existence?
- What is the structure of neutron stars and how do their properties depend on the underlying Hamiltonian?
- What role does pairing play in properties of neutron stars?

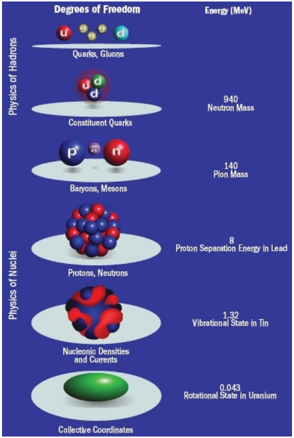


Fundamental Symmetries

- What explains the dominance of matter over antimatter in the universe?
- What is the nature of neutrinos and how do they interact with nuclei?
- Electric Dipole Moments of light nuclei?



Quantum Chromodynamics (QCD) is ultimately responsible for strong interactions: nucleons are the relevant degrees of freedom for low-energy nuclear physics→Nucleon-Nucleon potentials.



Nuclei are strongly-interacting many-body systems.

- What method do we use to solve the many-body Schrödinger equation?

$$H\,|\Psi\rangle = E\,|\Psi\rangle$$

$2^A \binom{A}{Z}$ coupled differential equations in $3A-3$ variables in the charge basis. (Can be lowered to $2^A \frac{2T+1}{A/2+T+1}\binom{A}{A/2+T}$ using an isospin-conserving basis).

^{4}He $\rightarrow$ 96 equations in 9 variables.
^{6}Li $\rightarrow$ 1 280 equations in 15 variables.
^{8}Be $\rightarrow$ 17 920 equations in 21 variables.
^{10}B $\rightarrow$ 258 048 equations in 27 variables.
^{12}C $\rightarrow$ 3 784 704 equations in 33 variables.
^{14}N $\rightarrow$ 56 229 888 equations in 39 variables.

- What is the Hamiltonian?

Green's function Monte Carlo (GFMC): the most accurate method for solving the many-body Schrödinger equation for light nuclei $4 < A \leq 12$.
First: Variational Monte Carlo.

- Guess a trial wave function Ψ_T. Generate a random position: $\mathbf{R} = \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A$.
- Metropolis algorithm: generate new positions $\mathbf{R}'$ based on the probability $P = \frac{|\Psi_T(\mathbf{R}')|^2}{|\Psi_T(\mathbf{R})|^2}$.
- Yields a set of "walkers" distributed according to the trial wave function. A walker: $\sum_\beta c_\beta \left|\mathbf{R}\beta\right\rangle$. $3A$ positions and $2^A\binom{A}{Z}$ spin/isospin states in the charge basis.
- Variational principle: $E_T = \frac{\langle\Psi_T|H|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle} \geq E_0$.

Second: Green's Function Monte Carlo.

- The wave function is imperfect: $|\Psi_T\rangle = \sum_{i=0}^{\infty} \alpha_i |\Psi_i\rangle$.
- Propagate in imaginary time to project out the ground state $|\Psi_0\rangle$:

$$|\Psi(t)\rangle = e^{-(H-\tilde{E}_0)t} |\Psi_T\rangle = e^{-(E_0-\tilde{E}_0)t} \left[\alpha_0 |\Psi_0\rangle + \sum_{i\neq 0} \alpha_i e^{-(E_i-E_0)t} |\Psi_i\rangle\right]$$

$$\Rightarrow \lim_{t\to\infty} |\Psi(t)\rangle \propto |\Psi_0\rangle .$$

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A cartoon

$$H = \frac{p_x^2}{2m} + V(x), \;\; V = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

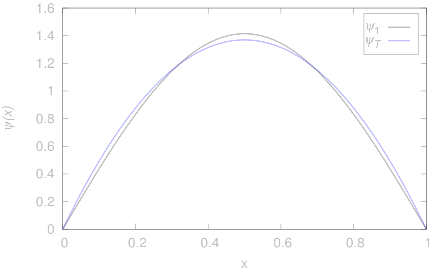
$$\hbar = m = L = 1$$

Solution

$$\psi_n(x) = \sqrt{2}\sin(n\pi x), \;\; E_n = \frac{n^2\pi^2}{2}.$$

"Trial wave function."

$$\psi_T(x) = -\sqrt{30}\left[\left(x - \frac{1}{2}\right)^2 - \frac{1}{4}\right].$$



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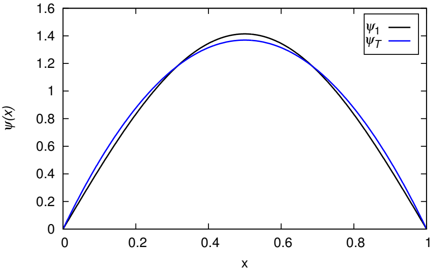
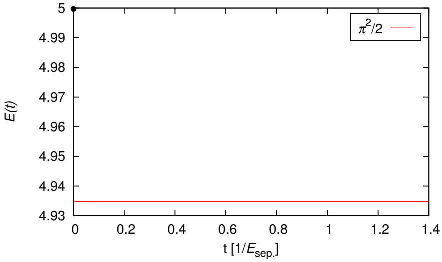
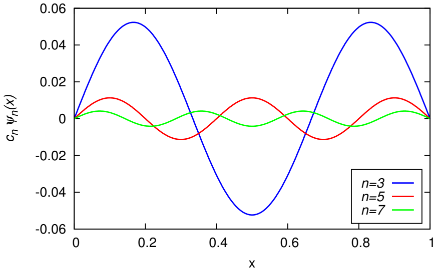


A cartoon

$$E(t) = \frac{\langle \psi_T | H e^{-(H-E_1)t} | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_1)t} | \psi_T \rangle}, \quad \psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x),$$

$$t = 0.0(1/E_{\mathrm{sep.}})$$





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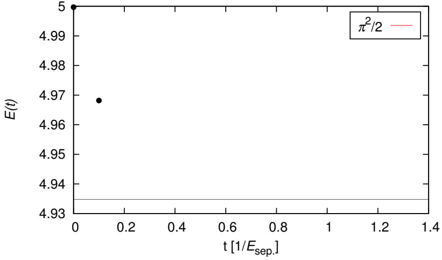

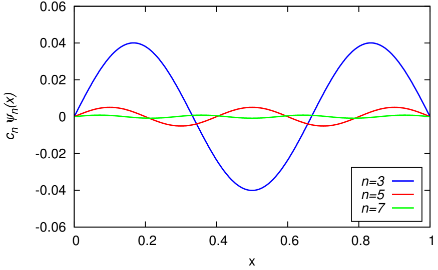

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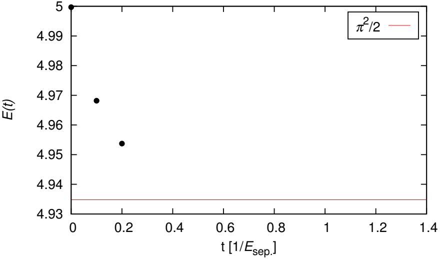
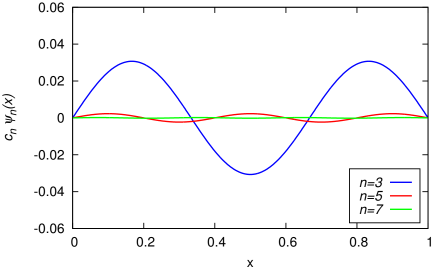
$$t = 0.2(1/E_{\text{sep.}})$$





A cartoon

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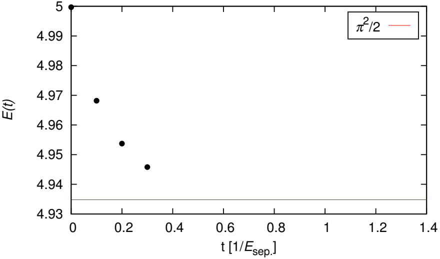
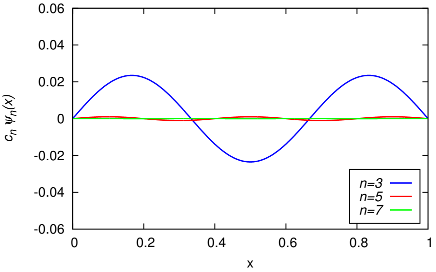
$$t = 0.3(1/E_{\text{sep.}})$$





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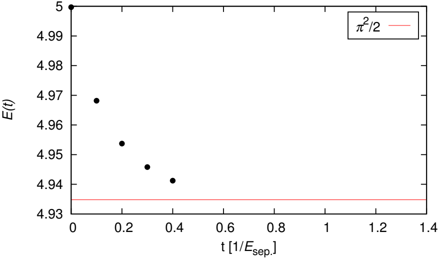
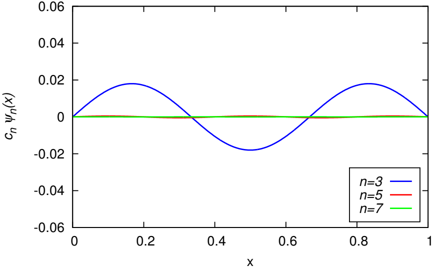
$$t = 0.4(1/E_{\mathrm{sep.}})$$

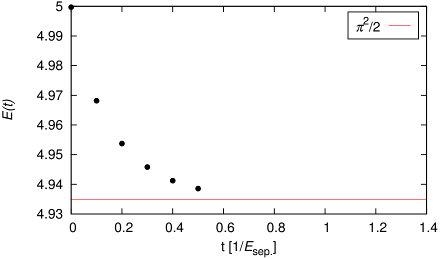


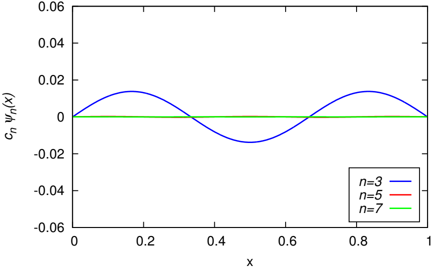


A cartoon

$$E(t) = \frac{\langle \psi_T | H e^{-(H-E_1)t} | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_1)t} | \psi_T \rangle}, \quad \psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x),$$

$$t = 0.5(1/E_{\text{sep.}})$$

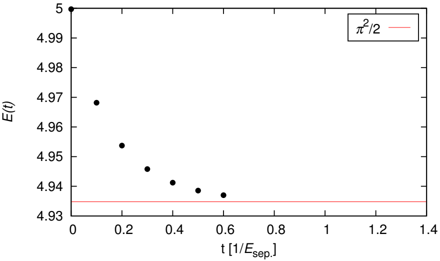


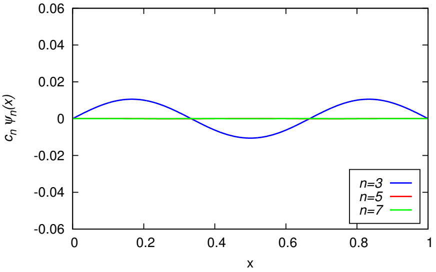


A cartoon

$$E(t) = \frac{\langle\psi_T|He^{-(H-E_1)t}|\psi_T\rangle}{\langle\psi_T|e^{-(H-E_1)t}|\psi_T\rangle}, \quad \psi_T(x) = \sum_{n=1}^{\infty} c_n\psi_n(x),$$

$$t = 0.6(1/E_{\text{sep.}})$$





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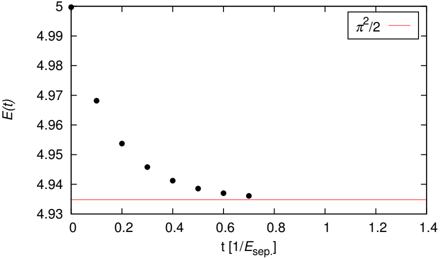
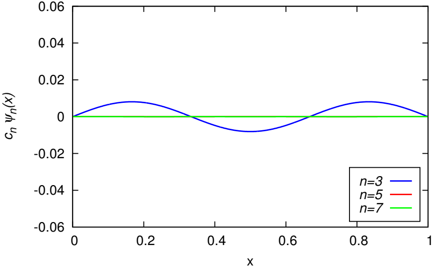
$$E(t) = \frac{\langle \psi_T | H e^{-(H-E_1)t} | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_1)t} | \psi_T \rangle}, \quad \psi_T(x) = \sum_{n=1}^{\infty} c_n \psi_n(x),$$

$$t = 0.7(1/E_{\mathrm{sep.}})$$





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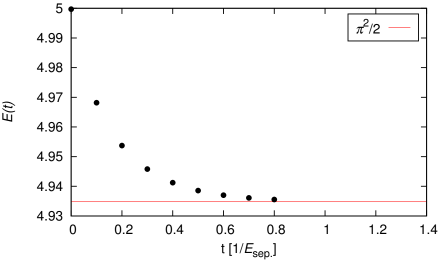
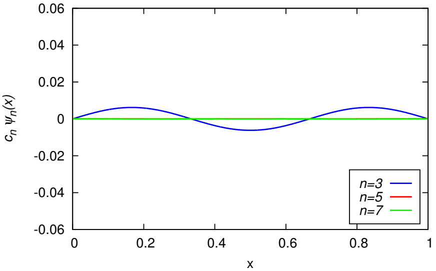
$$t = 0.8(1/E_{\text{sep.}})$$





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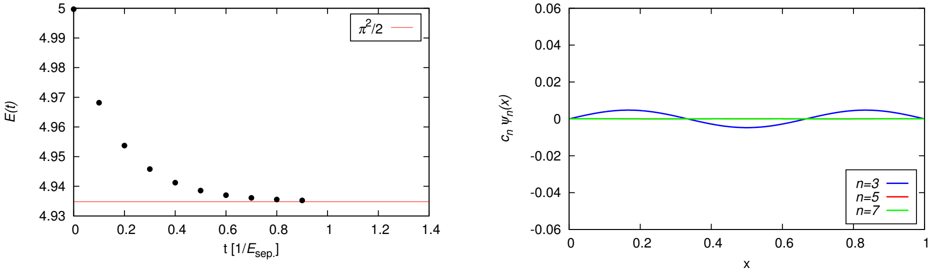
$$t = 0.9(1/E_{\text{sep.}})$$



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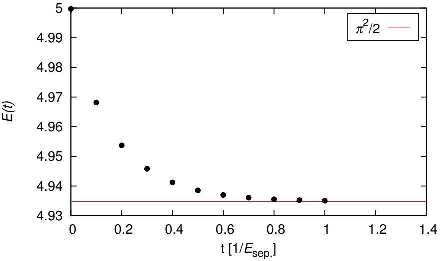
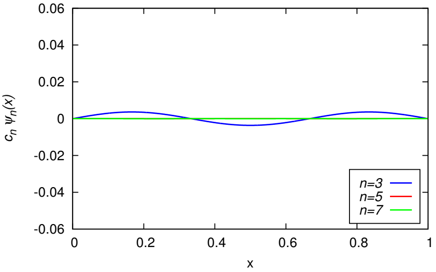
$$t = 1.0(1/E_{\text{sep.}})$$





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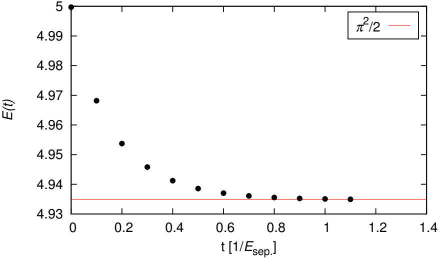

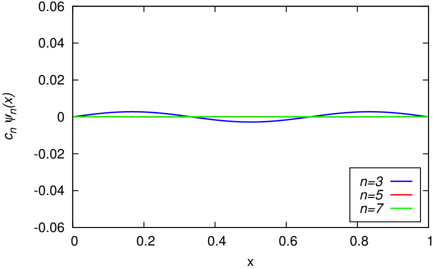

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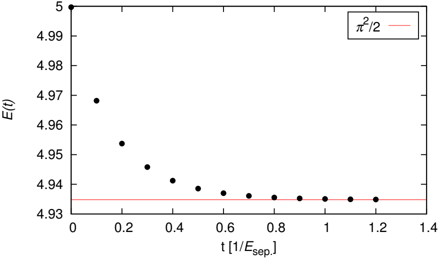

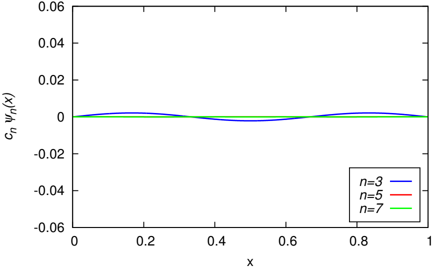

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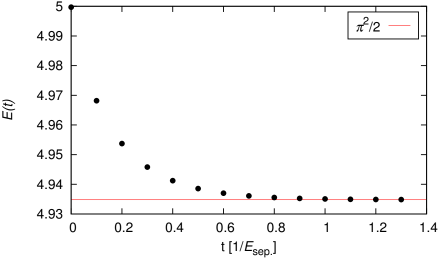
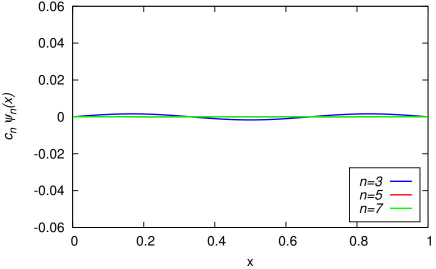
$$t = 1.3(1/E_{\text{sep.}})$$





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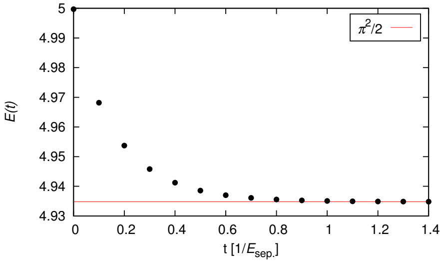
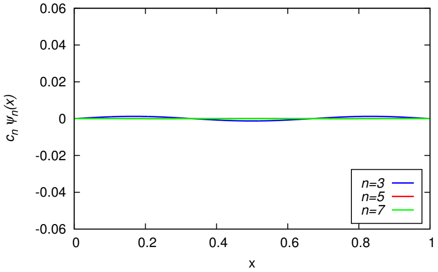
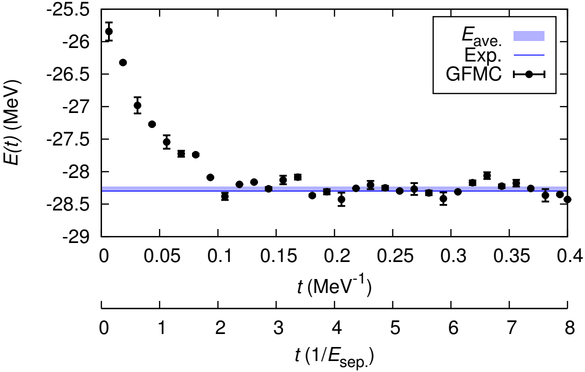
$$t = 1.4(1/E_{\text{sep.}})$$





For ^{4}He, $1/E_{\text{sep.}} = 1/|E_\alpha - E_t| \approx 0.05\ \text{MeV}^{-1}$.



Limitations

A walker consists of the $3A$ positions and $2^A\binom{A}{Z}$ spin-isospin states (in the charge basis).
^{12}C:$\rightarrow$Remember 3 784 704 spin-isospin states!

However: See some exciting work by S. Gandolfi, A. Lovato, J. Carlson, and Kevin E. Schmidt in auxiliary-field diffusion Monte Carlo (AFDMC)[1].

We can calculate "mixed estimates": $\frac{\langle\Psi(t)|O|\Psi_T\rangle}{\langle\Psi(t)|\Psi_T\rangle}$

$$\langle O(t)\rangle = \frac{\langle\Psi(t)|O|\Psi(t)\rangle}{\langle\Psi(t)|\Psi(t)\rangle} \approx \langle O(t)\rangle_{\text{Mixed}} + [\langle O(t)\rangle_{\text{Mixed}} - \langle O\rangle_T].$$

[1] arXiv:1406.3388 [nucl-th]

However...

For ground-state energies, $O = H$, and $[H, G] = 0$:

$$\langle H \rangle_{\text{Mixed}} = \frac{\langle \Psi_T | e^{-(H-E_T)t/2} H e^{-(H-E_T)t/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_T)t/2} e^{-(H-E_T)t/2} | \Psi_T \rangle}, \qquad \lim_{t\to\infty} \langle H \rangle_{\text{Mixed}} = E_0.$$

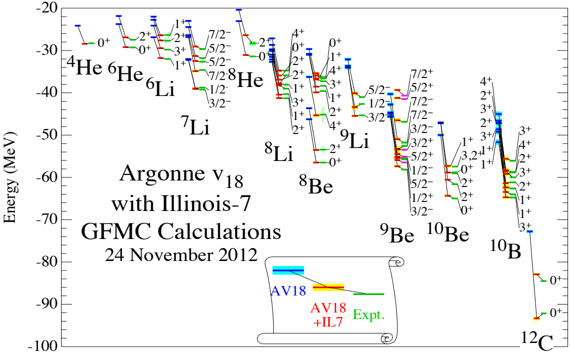
$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} V_{ijk} + \cdots$$

Until recently, there were two broad choices for v_{ij}.

- Local, real-space, phenomenological: Argonne v_{18}[2] - informed by theory, phenomenology, and experiment (well tested and very successful).
- Non-local, momentum-space, effective field theory (EFT): N^3LO[3] - informed by chiral EFT and experiment (well liked and often used in basis-set methods, such as the no-core shell model).

[2] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, PRC **51**, 38 (1995).
[3] e.g. D. R. Entem and R. Machleidt, PRC **68**, 041001 (2003)

Many excellent results using GFMC and phenomenological potentials [4].

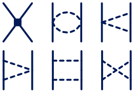
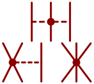
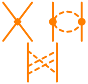


This is great! But... Until recently the nucleon-nucleon potentials used have been restricted to the phenomenological Argonne-Urbana/Illinois family of interactions.

[4] Figure courtesy of Steven C. Pieper and R. B. Wiringa

Background

Nuclear Interactions - Chiral EFT

		NN	NNN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^2LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^3LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

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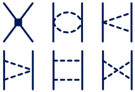
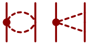
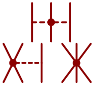
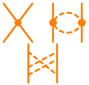
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

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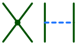
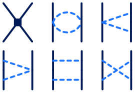
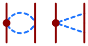
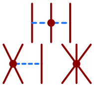
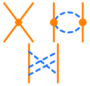
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

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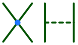
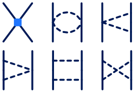
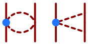
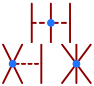
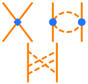
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
$\mathrm{N^2LO}$	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
$\mathrm{N^3LO}$	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

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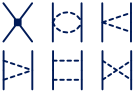
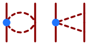
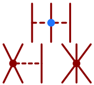
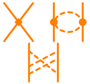
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

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Local construction possible[5] up to N^{2}LO.

Definitions.

$$\mathbf{q} = \mathbf{p} - \mathbf{p}', \ \mathbf{k} = \mathbf{p} + \mathbf{p}'$$

Regulator:

$$f(p, p') = e^{-(p/\Lambda)^n} e^{-(p'/\Lambda)^n}$$

$$\rightarrow f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4} : \ R_0 = 1.0, 1.1, 1.2 \text{ fm.}$$

Contacts:

$$\propto \mathbf{q} \text{ and } \mathbf{k}$$

$\rightarrow$ Choose contacts $\propto \mathbf{q}$ (As much as possible!)

[5] A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, PRC **90** 054323 (2014)

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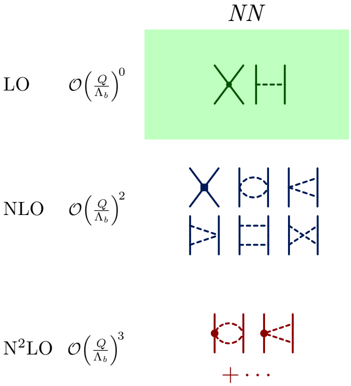
Background

Chiral EFT: Local Constructon Possible



$$V_{\text{cont.}}^{(0)} = \alpha_1 + \alpha_2(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + \alpha_3(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + \alpha_4(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$$

(Pauli exclusion principle) $\rightarrow$ Only two independent contacts!

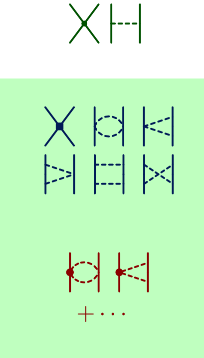
$$V_{\text{cont.}}^{(0)} = C_S + C_T(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)$$

NN

LO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$

NLO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$

N^{2}LO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$



$$
\begin{aligned}
V^{(2)}_{\text{cont.}} &= \gamma_1 q^2 + \gamma_2 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \\
&+ \gamma_3 q^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + \gamma_4 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\
&+ \gamma_5 k^2 + \gamma_6 k^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + \gamma_7 k^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\
&+ \gamma_8 k^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\
&+ (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\mathbf{q} \times \mathbf{k})(\gamma_9 + \gamma_{10}(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)) \\
&+ (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})(\gamma_{11} + \gamma_{12}(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)) \\
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\end{aligned}
$$

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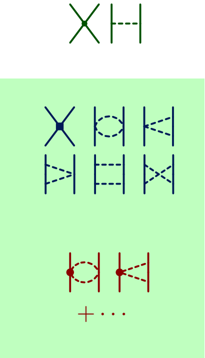

$$
\begin{aligned}
V_{\text{cont.}}^{(2)} &= \gamma_1 q^2 + \gamma_2 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \\
&+ \gamma_3 q^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + \gamma_4 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\
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\end{aligned}
$$

Local chiral EFT potential $\sim$ a v_7 potential

$$v_{ij} = \sum_{p=1}^{7} v_p(r_{ij}) O_{ij}^p + \sum_{p=15}^{18} v_p(r_{ij}) O_{ij}^p.$$

Charge-independent operators

$$O_{ij}^{p=1,14} = \left[1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}, \mathbf{L}\cdot\mathbf{S}, \mathbf{L}^2, \mathbf{L}^2(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j), (\mathbf{L}\cdot\mathbf{S})^2\right] \otimes \left[1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j\right].$$

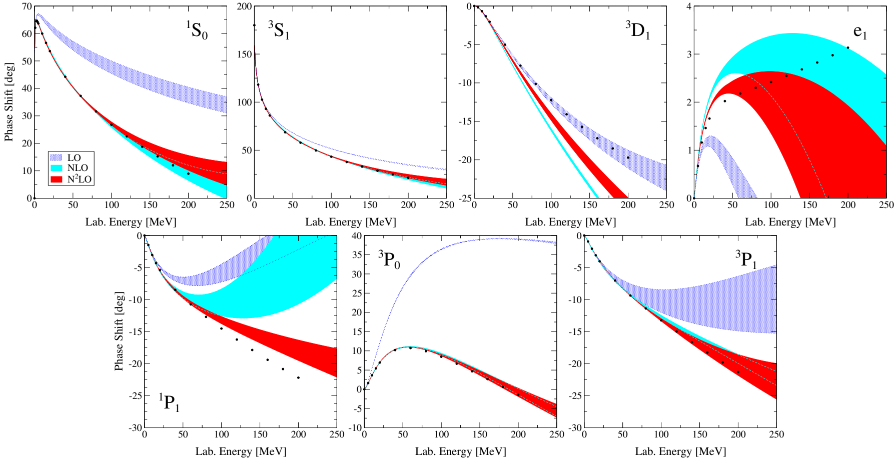
Charge-independence-breaking operators

$$O_{ij}^{p=15,18} = [1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes T_{ij}, \text{ and } (\tau_{zi} + \tau_{zj}).$$

Tensor operators

$$S_{ij} = 3(\boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}_{ij})(\boldsymbol{\sigma}_j \cdot \hat{\mathbf{r}}_{ij}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \; T_{ij} = 3\tau_{zi}\tau_{zj} - \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

Phase shifts for the *np* potential[6].



[6] A. Gezerlis et al. PRC **90** 054323 (2014)

NN Results[7]

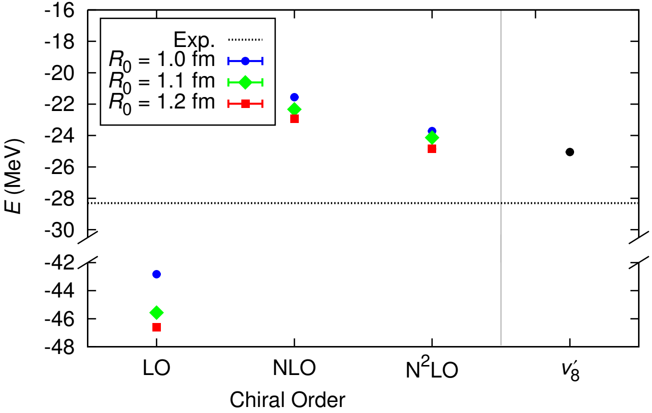
Investigate

- Theoretical uncertainties – Ground-state energies and radii at LO, NLO, and N^{2}LO
- Chiral convergence
  - Ground-state energies and radii at LO, NLO, and N^{2}LO
  - 1$^{\text{st}}$-order perturbation theory calculations for ^{4}He: $V_{\text{pert.}} = V_{\text{N}^2\text{LO}} - V_{\text{NLO}}$
  - 1$^{\text{st}}$-, 2$^{\text{nd}}$-, and 3$^{\text{rd}}$-order perturbation theory calculations for the deuteron
- Short-distance behavior – Contrast the short-distance (high-energy) features of one- and two-body distributions

[7] JEL, J. Carlson, E. Epelbaum, S. Gandolfi, A. Gezerlis, A. Schwenk, PRL **113** 192501 (2014)

Theoretical uncertainties & Chiral convergence

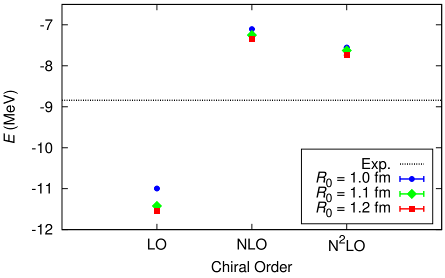
^{4}He ground-state energies at LO, NLO, and N^{2}LO: each with cutoff $R_0 = 1.0,\ 1.1,$ and 1.2 fm, compared with the value for AV8$'$.



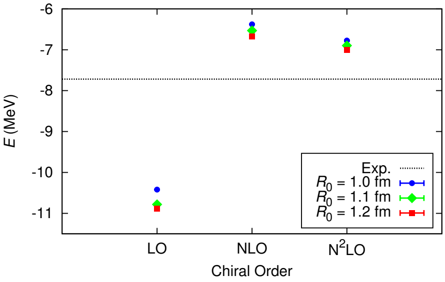
Theoretical uncertainties & Chiral convergence

^{3}H and ^{3}He ground-state energies at LO, NLO, and N^{2}LO: each with cutoff $R_0 = 1.0,\ 1.1,$ and 1.2 fm.

^{3}H

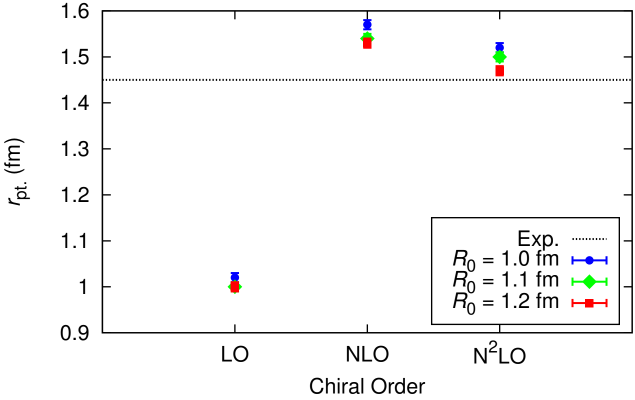


^{3}He



Theoretical uncertainties & Chiral convergence

^{4}He point proton radii – $r^2_{\text{pt.}} = r^2_{\text{ch.}} - r^2_p - \frac{N}{Z} r^2_n$ (IA) at LO, NLO, and N^{2}LO: each with cutoff $R_0 = 1.0,\ 1.1,$ and 1.2 fm.



NN Results

$A = 3$ Radii - $\langle r^2_{\text{pt.}} \rangle^{1/2}$

Theoretical uncertainties & Chiral convergence

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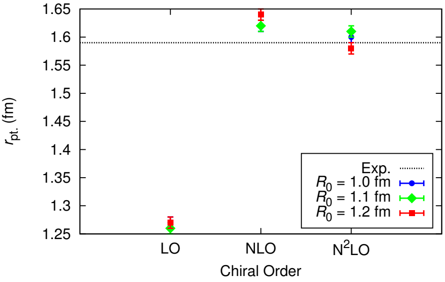
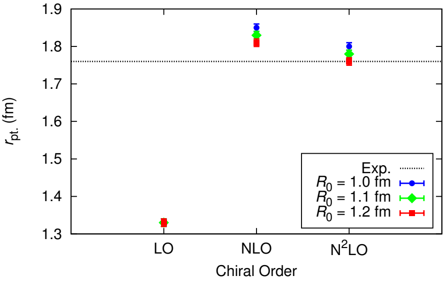
^{3}H



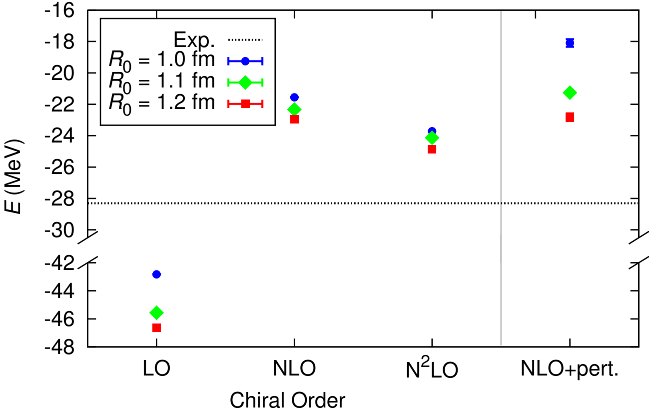
^{3}He



Chiral convergence

^{4}He ground-state energy in first-order perturbation theory.

$E_{\mathrm{NLO}} + \langle \Psi_{\mathrm{NLO}} | V_{\mathrm{pert.}} | \Psi_{\mathrm{NLO}} \rangle$, with $V_{\mathrm{pert.}} = V_{\mathrm{N^2LO}} - V_{\mathrm{NLO}}$.



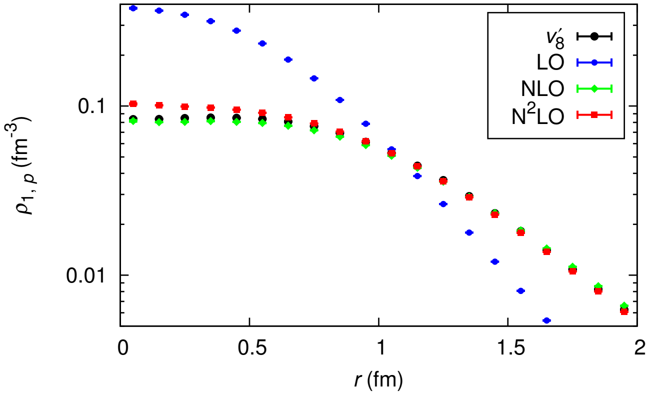
Chiral convergence

- Write $H \rightarrow \langle k' J M_J L' S | H | k J M_J L S\rangle$.
- Diagonalize$\rightarrow \{\psi_D^{(i)}(r)\}$.
- Second- and third-order perturbation theory calculations for ^{2}H possible.

Calculation	E (MeV) $R_0 = 1.0$ fm	$R_0 = 1.1$ fm	$R_0 = 1.2$ fm
E_{NLO}	-2.15	-2.16	-2.16
$E_{\mathrm{NLO}} + V^{(1)}_{\mathrm{pert.}}$	-1.44	-1.80	-1.90
$E_{\mathrm{NLO}} + V^{(2)}_{\mathrm{pert.}}$	-2.11	-2.17	-2.18
$E_{\mathrm{NLO}} + V^{(3)}_{\mathrm{pert.}}$	-2.13	-2.18	-2.19
$E_{\mathrm{N^2LO}}$	-2.21	-2.21	-2.20

Short-distance behavior

Proton distribution: $\rho_{1,p}(r) = \frac{1}{4\pi r^2}\langle\Psi|\sum_i \frac{1+\tau_z(i)}{2}\delta(r - |\mathbf{r}_i - \mathbf{R}_{\text{c.m.}}|)|\Psi\rangle.$

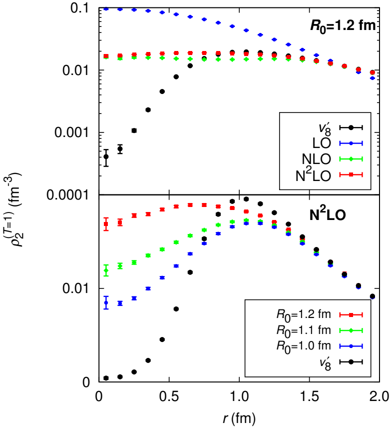


NN Results

Two-Body $T = 1$ Distribution - ^{4}He

Short-distance behavior

Two-body $T = 1$ distribution: $\rho_2^{(T=1)}(r) = \frac{1}{4\pi r^2} \langle \Psi | \sum_{i<j} \frac{3+\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j}{4} \delta(r - |\mathbf{r}_{ij}|) | \Psi \rangle.$



NNN Interaction[8]

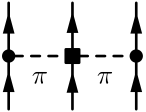
Investigate

- The form of the force – Fourier transforming, regulating, some ambiguity.
- Fitting c_D and c_E – ^{4}He binding energy and n-α scattering phase shifts.
- Results for Light Nuclei – $A \leq 4$ radii and binding energies.

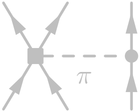
[8] Current work

NNN Interaction

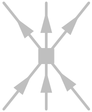
The Form of the Force – Momentum Space



c_1, c_3, c_4



c_D



c_E

$$V_C = \frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2 \sum_{\pi(ijk)} \frac{(\boldsymbol{\sigma}_i \cdot \mathbf{q}_i)(\boldsymbol{\sigma}_j \cdot \mathbf{q}_j)}{(\mathbf{q}_i^2 + m_\pi^2)(\mathbf{q}_j^2 + m_\pi^2)} F_{ijk}^{\alpha\beta} \tau_i^\alpha \tau_j^\beta,$$

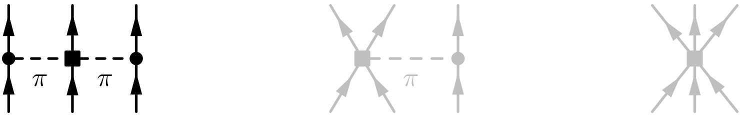
$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta}\left[-\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2}(\mathbf{q}_i \cdot \mathbf{q}_j)\right] + \frac{c_4}{f_\pi^2}\epsilon^{\alpha\beta\gamma}\tau_k^\gamma[\boldsymbol{\sigma}_k \cdot (\mathbf{q}_i \times \mathbf{q}_j)],$$

$$V_D = -\frac{g_A}{8f_\pi^2}\frac{c_D}{f_\pi^2\Lambda_\chi} \sum_{\pi(ijk)} \frac{\boldsymbol{\sigma}_j \cdot \mathbf{q}_j}{\mathbf{q}_j^2 + m_\pi^2}(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)(\boldsymbol{\sigma}_i \cdot \mathbf{q}_j),$$

$$V_E = \frac{c_E}{2f_\pi^4\Lambda_\chi} \sum_{i \neq j} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j.$$

NNN Interaction

The Form of the Force – Momentum Space



c_1, c_3, c_4 $\qquad$ c_D $\qquad$ c_E

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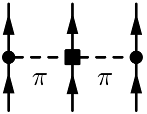
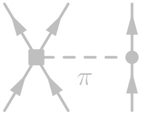
NNN Interaction

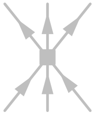
The Form of the Force – Momentum Space



c_1, c_3, c_4



c_D



c_E

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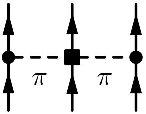
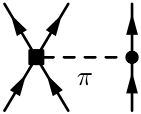
NNN Interaction

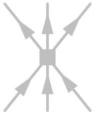
The Form of the Force – Momentum Space



c_1, c_3, c_4



c_D



c_E

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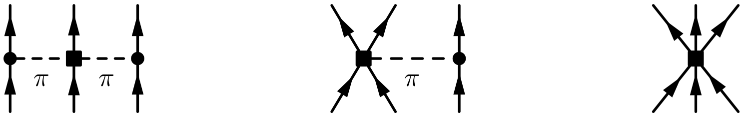

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$$V_E = \frac{c_E}{2f_\pi^4\Lambda_\chi} \sum_{i\neq j} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j.$$

NNN Interaction

The Form of the Force – Definitions

$$\mathcal{F}\left\{ i \;\bullet\!\!\underset{\pi}{-\,-\,-}\!\!\bullet\; j \right\} \rightarrow \; X_{ij}(\mathbf{r}_{ij})$$

where

$$X_{ij}(\mathbf{r}_{ij}) = S_{ij}(\mathbf{r}_{ij})\, T(r_{ij}) + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\, Y(r_{ij}),$$

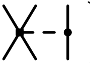
$$T(r) = \left(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2}\right) Y(r),$$

$$Y(r) = \frac{\exp\left(-m_\pi r\right)}{m_\pi r}\left(1 - e^{-(r/R_0)^4}\right),$$

$$\delta^{(3)}(\mathbf{r}_{ij}) \rightarrow \Delta_{ij} \equiv \frac{1}{\pi \Gamma(3/4) R_0^3} \exp(-(r_{ij}/R_0)^4).$$

NNN Interaction

The Form of the Force – Real Space: 1π-Exchange + Contact

$$\mathcal{F}\Big\{$$  $$\Big\} \rightarrow 1\pi\text{-Exchange} + \text{Contact}$$

c_D

Some ambiguity here: which nucleons are participating in the pion exchange? Two possible short-range structures.

$$A^{1\pi+C} \sum_{i<j<k} \sum_{\text{cyc.}} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k) \left[X_{ik} - \frac{2^2\pi}{m_\pi^3} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k) \Delta_{ik} \right] (\Delta_{ij} + \Delta_{kj})$$

or

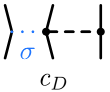
$$A^{1\pi+C} \sum_{i<j<k} \sum_{\text{cyc.}} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k) \left[X_{ik}(\mathbf{r}_{kj}) \Delta_{ij} + X_{ik}(\mathbf{r}_{ij}) \Delta_{kj} - \frac{2^3\pi}{m_\pi^3} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k) \Delta_{ij} \Delta_{kj} \right]$$

$$A^{1\pi+C} = \frac{g_A \, c_D \, m_\pi^3}{2^5 3\pi \Lambda_\chi f_\pi^4}$$

NNN Interaction

The Form of the Force – Real Space: 1π-Exchange + Contact

$$\lim_{m_\sigma \to \infty} \mathcal{F}\Big\{$$



$$\Big\} \to 1\pi\text{-Exchange} + \text{Contact}$$

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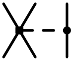
NNN Interaction

The Form of the Force – Real Space: 1π-Exchange + Contact

$$\mathcal{F}\left\{ \quad \right\} \rightarrow 1\pi\text{-Exchange} + \text{Contact}$$



c_D

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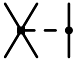
NNN Interaction

The Form of the Force – Real Space: 1π-Exchange + Contact

$\mathcal{F}\Big\{$  $\Big\} \to 1\pi$-Exchange + Contact

c_D

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Two possible short-range structures.

$$A^{1\pi+C} \sum_{i<j<k} \sum_{\text{cyc.}} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k) \left[X_{ik} - \frac{2^2\pi}{m_\pi^3} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k) \Delta_{ik} \right] (\Delta_{ij} + \Delta_{kj})$$

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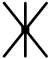
NNN Interaction

The Form of the Force – Real Space: Contact

$\mathcal{F}\Big\{$  $\Big\} \to$ Contact

c_E

The same ambiguity here:

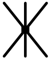
$$A^C \sum_{i<j<k} \sum_{\text{cyc.}} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k)\Delta_{ij}\Delta_{kj}$$

$$\frac{A^C}{2} \sum_{i<j<k} \sum_{\text{cyc.}} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k)\Delta_{ij}(\Delta_{kj} + \Delta_{ik})$$

$$A^C = \frac{c_E}{\Lambda_\chi f_\pi^4}$$

NNN Interaction

The Form of the Force – Real Space: Contact

$\mathcal{F}\Big\{$  $\Big\} \to$ Contact

c_E

The same ambiguity here:

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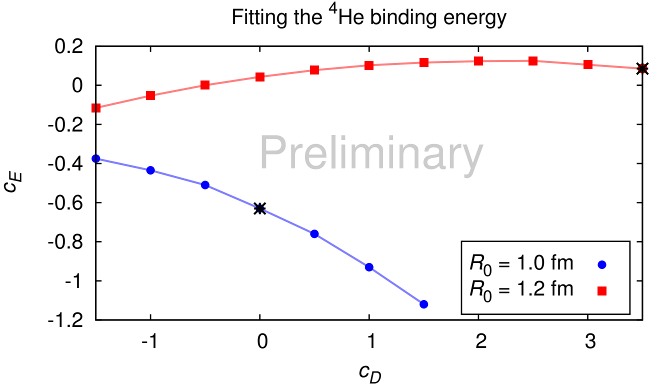
$$\cancel{\frac{A^C}{2} \sum_{i<j<k} \sum_{\text{cyc.}} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k)\Delta_{ij}(\Delta_{kj} + \Delta_{ik})}$$

$$A^C = \frac{c_E}{\Lambda_\chi f_\pi^4}$$

What to fit c_D and c_E to?

- Uncorrelated observables.
- Probe properties of light nuclei: ^{4}He E_B.
- Probe $T = 3/2$ physics: n-α scattering phase shifts.

Curves of c_E vs. c_D, fitting to ^{4}He E_B.



For low-energy scattering and one open channel of total angular momentum J,

$$\Psi \propto \{\Phi_{c_1}\Phi_{c_2} Y_L\}_J \left[\cos\delta_{JL} j_L(kr_c) - \sin\delta_{JL} n_L(kr_c)\right],$$

Impose[9]

$$\hat{\mathbf{n}} \cdot \boldsymbol{\nabla}_{\mathbf{r}_c} \Psi = \gamma \Psi \text{ at } r_c = R_0$$

$$\Rightarrow \tan\delta_{JL} = \frac{\gamma j_L(kR_0) - k j_L'(kR_0)}{\gamma n_L(kR_0) - k n_L'(kR_0)}$$

[9] Kenneth M. Nollet, Steven C. Pieper, R. B. Wiringa, J. Carlson, G. M. Hale, PRL **99**, 022502 (2007)

Reject samples with $r_c > R_0$, but

$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}_c|<R_0} d\mathbf{R}_{c_1}\, d\mathbf{R}_{c_2}\, d\mathbf{r}_c\, G(\mathbf{R}', \mathbf{R}; \Delta t)\Psi_n(\mathbf{R}) + \int_{|\mathbf{r}_e|>R_0} d\mathbf{R}_{c_1}\, d\mathbf{R}_{c_2}\, d\mathbf{r}_c\, G(\mathbf{R}', \mathbf{R}; \Delta t)$$

maps to

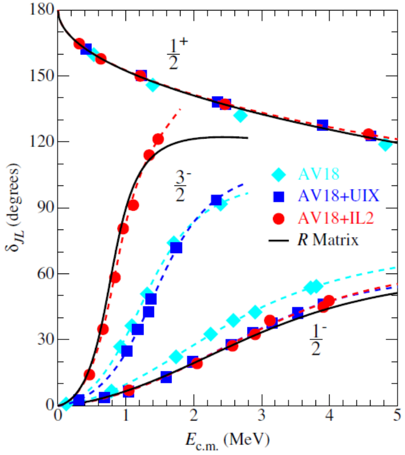
$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}|<R_0} d\mathbf{R}_{c_1}\, d\mathbf{R}_{c_2}\, d\mathbf{r}_c\, G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R}) \times \left[\Psi_n(\mathbf{R}) + \frac{G(\mathbf{R}', \mathbf{R}_e; \Delta\tau)}{G(\mathbf{R}', \mathbf{R}; \Delta\tau)} \left(\frac{r_e}{r_c}\right)^3 \Psi_n(\mathbf{R}_e)\right]$$

The wave function at the $(n+1)$th Δt step gets a contribution from the previous point $\mathbf{R}$ and an "image" point at $\mathbf{R}_e$.

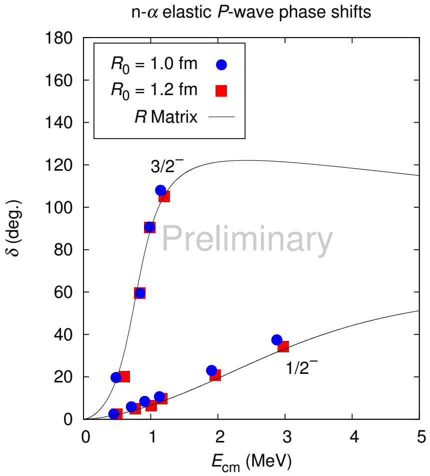
NNN Interaction

Current Work - ^{5}He Fit

Results showed the need for greater spin-orbit splitting than was provided by the largely Fujita-Miyazawa-like UIX NNN interaction.

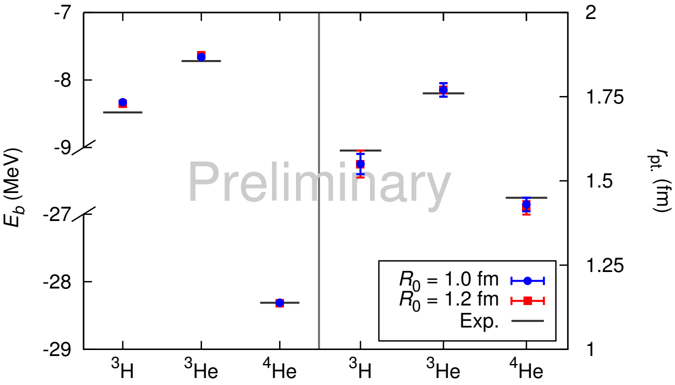


^{5}He fit to $P3/2^-$ wave. R-matrix analysis provided by G. M. Hale.



NNN Interaction

Current Work - Results for Light Nuclei



Conclusion

Summary

- Low-energy nuclear theory: QMC+χEFT may help answer many interesting questions in physics.
- Phenomenological potentials have been very successful but there are compelling reasons to investigate and compare them to chiral EFT interactions.
- **GFMC calculations of light nuclei are now possible with chiral EFT interactions.**
- The softest of the potentials with $R_0 = 1.2$ fm is more perturbative in the difference between N^{2}LO and NLO.
- The high-momentum (short-range) behavior of chiral EFT interactions is distinct from the phenomenological interactions.
- **The consistent 3N interaction at N^{2}LO appears to be able to fit simultaneously properties of light nuclei and n-α scattering phase shifts.**

Conclusion

Future Work

- Include 2-nucleon force at N^{3}LO (which will be partly non-local).
- Extend to larger nuclei with $4 < A \leq 12$: compare with Argonne+Illinois results.
- Derive and implement electroweak currents in a consistent chiral EFT framework.
- Include Δ-full N^{3}LO NN chiral EFT interaction of M. Piarulli et al. in GFMC. Derive and implement consistent 3N interaction.
- Extend n-α scattering framework to other (multichannel?) reactions, e. g. n-$\alpha \to d + t$.
- Investigate the role of pairing correlations in AFDMC calculations of neutron matter with small proton fractions and what effect this has on neutron-star properties.
- Parity- and CP-violating observables: Electric dipole moments of light nuclei: ^{6}Li?

Los Alamos National Laboratory:

S. Gandolfi, J. Carlson

University of Guelph:

A. Gezerlis

Technische Universität Darmstadt:

A. Schwenk, I. Tews

Universität Bochum:

E. Epelbaum

NERSC

NUCLEI

Nuclear Computational Low-Energy Initiative

Thank you!

The trial wave function is a symmetrized product of correlation operators acting on a Jastrow wave function.

Trial Wave Function

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j}(1+U_{ij})\right]|\Psi_J\rangle\ ,$$

$$U_{ij} = \sum_{p=2}^{m} u_p(r_{ij})\,O^p_{ij},\ \ |\Psi_J\rangle = \prod_{i<j} f_c(r_{ij})\,|\Phi_A\rangle\ ,$$

$$|\Phi_4\rangle = \mathcal{A}\,|p\!\uparrow\, p\!\downarrow\, n\!\uparrow\, n\!\downarrow\rangle\ ,$$

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j}(1+u_\sigma(r_{ij})\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j + u_{t\tau}(r_{ij})S_{ij}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)\right]\prod_{i<j} f_c(r_{ij})\,|\Phi_4\rangle$$

NN Results

^{4}He Binding Energies - $\langle H \rangle$

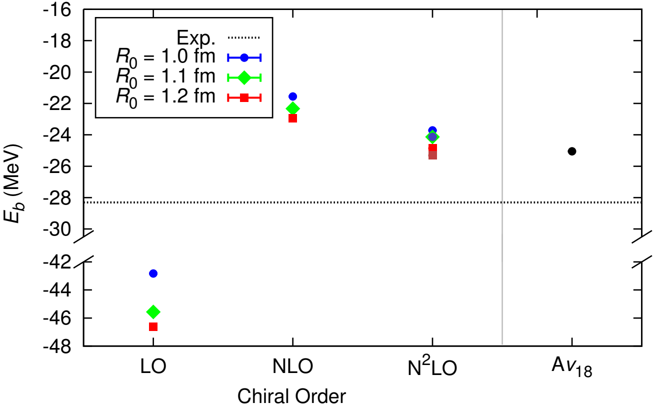


Figure: ^{4}He binding energy at different chiral orders and cutoff values. SFR dependence weak.